

Stochastic solution of nonlinear and nonhomogeneous evolution problems by a differential Kolmogorov equation

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Abstract

A large class of physically important nonlinear and nonhomogeneous evolution problems, characterized by advection-like and diffusion-like processes, can be usefully studied by a time-differential form of Kolmogorov's solution of the backward-time Fokker-Planck equation. The differential solution embodies an integral representation theorem by which any physical or mathematical entity satisfying a generalized nonhomogeneous advection-diffusion equation can be calculated incrementally in time. The utility of the approach for tackling nonlinear problems is illustrated via solution of the noise-free Burgers and related Kardar-Parisi-Zhang (KPZ) equations where it is shown that the differential Kolmogorov solution encompasses, and allows derivation of, the classical Cole-Hopf

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and KPZ transformations and solutions. A second example, illustrating application of this approach to nonhomogeneous evolution problems, derives the Feynman-Kac formula appropriate to a Schrödinger-like equation.

Key words. nonlinear partial differential equations, stochastic methods, Cole-Hopf transformation, Feynman-Kac formula

AMS subject classifications. 82C31, 35K55, 60H30

Abbreviated title. Stochastic solution of evolution equations

1. Introduction

A wide array of physically important time-evolutionary problems, in areas as diverse as hydrodynamic turbulence [1–3], quantum mechanics [4, 5], and the evolution of cosmic large-scale structure [6], can be modeled by nonlinear equations of the generic form

$$\eta_\theta + \mathbf{b} \cdot \nabla \eta + \nu \nabla^2 \eta = f(\eta, \eta_i, \eta_{ij} \dots n) \quad (1)$$

where η represents a scalar field whose evolution within a finite or non-finite space-time domain is determined, at least in part, by processes that in some fashion, are analogous to advection and/or molecular diffusion within a hydrodynamic flow. Here, \mathbf{b} and ν correspond to, or are analogs of, the local dimensional or nondimensional drift field and diffusion coefficient, respectively, while the source term, f , can include linear and nonlinear terms in both η and derivatives of η up to order n . In addition, since we will conceptualize the incremental, stochastic construction of η as

a procedure in which random walkers are launched from a space-time solution point (\mathbf{x}, θ) toward known/previously calculated η , we will follow Kolmogorov and state the evolution of η in terms of backward time, θ .

It is well known, particularly in the applied mathematics community [7, 8] that *linear* models, which are encompassed by (1), can be solved over finite (non-incremental) time intervals via application of Kolmogorov's solution of the backward-time Fokker Planck (FP) equation. In cases where (1) has either a nonlinear or linear source term, f , in η , or a drift \mathbf{b} and/or diffusivity dependent on η (where the latter can arise in more general forms of the third term on the left of (1)), a Kolmogorov solution can still be *expressed* in representative or schematic form [9, 10]; however, in these instances, one or more stochastic path integrals in the *a priori* unknown scalar field, $\eta(\mathbf{x}, \theta)$, appear. While one can, in principal, formulate a system of equations in the unknown η , and attempt a numerical solution over the entire space-time domain, Q , this is computationally expensive and apparently remains untried. Here, we focus on simpler, low cost, and often analytically tractable local solutions.

The purpose of this paper is to point up the utility of applying a *time-differential* version of Kolmogorov's solution to nonlinear and nonhomogeneous evolution problems of the form in (1). In order to demonstrate the potential of this approach for tackling nonlinear problems, we show how the differential Kolmogorov solution can be used to derive the Cole-Hopf and related Kardar-Parisi-Zhang (KPZ) solutions of the noise-free Burger's [11, 12] and KPZ [13] equations. We then apply this approach to nonhomogeneous problems, deriving the Feynman-Kac formula as a solution to a Schrödinger-like equation. We find that, at least in these test cases, the differential

Kolmogorov solution offers an alternative, relatively straightforward, physically transparent basis for solution. Moreover, since this approach can be adapted to accommodate the effects of boundary interactions/boundary conditions on the evolution of η [14] (see also the caption to Fig. 2), the potential for further applications seems clear.

Our jumping-off point is thus Kolmogorov's solution of the backward-in-time Fokker-Planck equation, connecting the stochastic kinematics of random walkers within a finite or non-finite space-time region, $Q = D \times (\theta, T]$, to the evolution of the scalar field, $\eta(\mathbf{x}, \theta)$, within Q . Here, D is the spatial domain, $\theta = T - t$, is again backward time, t forward time, and T the forward time at which a solution for $\eta(\mathbf{x}, \theta)$ is sought. The solution, written here for finite Q , and represented schematically in Fig. 1, reads [7] :

$$\eta(\mathbf{x}, \tilde{\theta}) = E_{\mathbf{x}, \tilde{\theta}}[g(\chi(\tau), \tau)] + E_{\mathbf{x}, \tilde{\theta}}[\phi(\chi(\tau))] - E_{\mathbf{x}, \tilde{\theta}}\left[\int_{\tilde{\theta}}^{\tau} f(\chi(s), s) ds\right] \quad (2)$$

where the first two terms on the right capture the effects of the random walker (RW) swarm, launched from the solution point $(\mathbf{x}, \tilde{\theta})$, sampling (typically known) Dirichlet conditions, $\eta = g(\mathbf{x}, \theta')$, on the boundary δQ of Q , and the final condition $\eta = \phi(\mathbf{x}, \theta = T)$ on the final time-slice, $D \times \{\theta = T\}$. In cases where Neumann and/or mixed conditions are imposed on δQ , an additional term similar to the first appears [14]. Throughout, E will represent the expectation taken with respect to the solution point. In addition, in (2), τ represents the random time at which any given RW impinges either on δQ (first term on right side of (2)), or on $D \times \{\theta = T\}$ (second term).

Couching the development mainly in hydrodynamic terms, and depicting the time-incremental

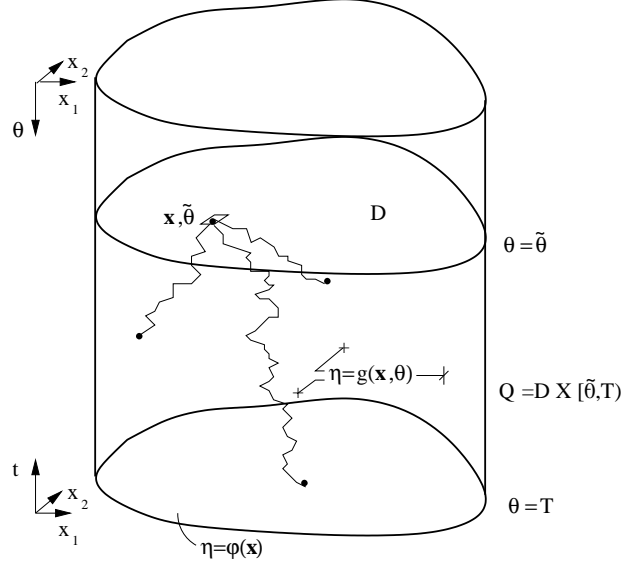


Figure 1: Kolmogorov's local, non-time-incremental stochastic construction of the scalar $\eta(\mathbf{x}, \tilde{\theta})$, as given by Eq. (2), appropriate to linear versions of Eq. (1), where the drift, \mathbf{b} , and diffusivity, ν (or their non-hydrodynamic analogs) are known. In this illustration, η is subject to the Dirichlet condition $\eta = g(\mathbf{x}, \theta)$ on the boundary δQ of the space-time cylinder Q , while on the final-time slice, $D \times \{\theta = T\}$, $\eta = \phi(\mathbf{x})$.

solution in Fig. 2, we focus below on a differential form of (2), expressed over short backward time intervals, $\Delta\theta = \theta_{j+1} - \theta_j$, where $\Delta\theta$ is chosen so that the magnitudes of all three terms on the left side of (1) remain comparable over the interval. This is an important point both physically and computationally and translates to the condition $|(\mathbf{x} - \bar{\mathbf{x}}(\theta_{j+1}))|^2/l_D^2 \approx [b(x, \theta_j)\Delta\theta]^2/(\nu\Delta\theta) = bl_b/\nu = O(1)$, where $b = |\mathbf{b}(\mathbf{x}, \theta)|$, $\mathbf{b}(\mathbf{x}, \theta_j) = -\mathbf{u}(\mathbf{x}, \theta_j)$ is the local drift, $l_D = \sqrt{\nu\Delta\theta}$ is the local diffusion length scale, $l_b = b\Delta\theta$ is the local advection length scale, and $\bar{\mathbf{x}}(\theta_{j+1})$ is the mean position of the random walk swarm at θ_{j+1} . [Note, $\bar{\mathbf{x}}(\theta_{j+1}) = \mathbf{x} + E \int_{\theta_j}^{\theta_{j+1}} \mathbf{b}(\chi(s'))ds' = \mathbf{x} + \mathbf{b}(\mathbf{x}, \theta_j)\Delta\theta + O(\Delta\theta^2)$].

Thus, in hydrodynamic terms, we arrive at the requirement that $\Delta\theta$ must be chosen so that the local Reynolds number, $Re = bl_b/\nu$, remains order 1, or more meaningfully, so that the local

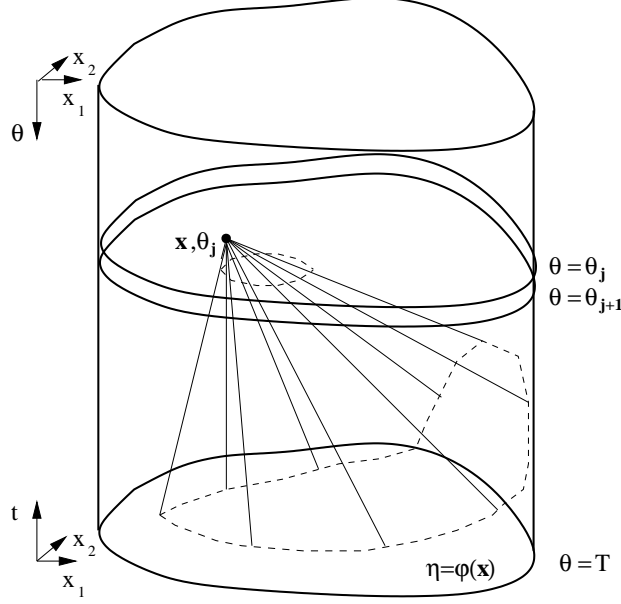


Figure 2: Incremental stochastic construction of $\eta(\mathbf{x}, \theta_j)$, appropriate to nonlinear versions of Eq. (1). Here, an approximate 'cone-of-influence' is shown, indicating how the local solution at (\mathbf{x}, θ_j) would typically depend on previously determined η , computed incrementally over $[\theta_{j+1}, T)$. In this illustration, a drift field (or drift field analog), \mathbf{b} , having a significant x_1 component, pushes RW's predominantly to the right. Near Dirichlet boundaries, RW impingement with a boundary element $\delta Q_k = \delta D \times \Delta\theta_k$ (where δD is the boundary of D and $\Delta\theta_k = \theta_{k+1} - \theta_k$), is readily accommodated using the first expectation in Eq. (2), applied over δQ_k . A similar (or additional) term would be required near Neumann (or mixed) boundaries [14].

advection length scale, $l_b = b\Delta\theta$, is on the order of the local diffusion length scale, l_D . More importantly, this condition implies that non-fixed time steps may, under various circumstances, be required in both analytical [14] and Monte Carlo solutions, a point recognized in the applied math literature [15], but apparently not well known in the engineering and physics communities.

In order to allow comparisons with known results, we will: i) assume that the solution point $(\mathbf{x}, \theta) \in Q$ is sufficiently removed from boundaries to allow neglect of boundary interaction effects, and ii) focus on one-dimensional problems. The method to be described carries over without

difficulty to multiple dimensions, and as noted, can be adapted to handle boundary conditions. In addition, for notational simplicity, we will set $\nu = 1$; based on the discussion immediately above, this corresponds to nondimensionalizing (1) using l_b (or equivalently, l_D), b , and $\Delta\theta$ for the length, drift, and time scales, respectively, and then to setting $Re_b = 1$.

Thus, we express the time-differential form of (2) in either of two equivalent forms:

$$\eta(x, \theta_j) = \int_{-\infty}^{\infty} p(x, \theta_j | x', \theta_{j+1}) \eta(x', \theta_{j+1}) dx' - E \int_{\theta_j}^{\theta_{j+1}} f(\chi(s'), s') ds' \quad (3)$$

or

$$\eta(x, \theta_j) \approx \sum_{i=1}^{N_x} \left[\frac{n(x'_i, \theta_{j+1})}{N} \right] \eta(x'_i, \theta_{j+1}) - \frac{1}{N} \sum_{k=1}^N \int_{\theta_j}^{\theta_{j+1}} f(\chi_k(s'), s') ds' \quad (4)$$

where p is the transition density, $n(x'_i, \theta_{j+1})/N$ is the fraction of N RW's launched from the solution point (x, θ_j) reaching a line segment, Δx_i (on the x-axis), during the interval $(\theta_j, \theta_{j+1}]$, $x'_i \in \Delta x_i$, and N_x is the number of increments used to discretize a length $2L$ of the x-axis. Here, $2L$ is, e.g., centered on x , and L is chosen to be much larger than the maximum RW displacement produced by combined advection and diffusion over $\Delta\theta$.

With regard to the differential solutions in (3) and (4), we note that (3) is useful when the transition density, p , can be determined analytically via the FP equation; this approach is illustrated in our derivation of the Cole-Hopf/KPZ (CH/KPZ) transformation below. The second form, (4), which is useful, for example, in Monte Carlo simulations where analytical p 's are not available, is based on the following simple relationship between p and the fraction $n(x'_i, \theta_{j+1})/N$: $p(x, \theta_j | x'_i, \theta_{j+1}) = \lim_{\Delta x_i \rightarrow 0} n(x'_i, \theta_{j+1})/(N \Delta x_i)$. As a practical aside, and considering (4), the frac-

tions $n(x'_i, \theta_{j+1})/N$ are obtained by launching a swarm of N RW's from the solution point (x, θ_j) , and then by counting the number of RW's that subsequently reach each Δx_i over the increment $(\theta_j, \theta_{j+1}]$.

With regard to the path integral terms in (3) and (4), these can be expressed, depending on the application, as $f(x, \theta_{j+1})\Delta\theta + O(\Delta\theta^2)$, or $f(x, \theta_j)\Delta\theta + O(\Delta\theta^2)$. This point is exploited in our derivation of the Feynman-Kac formula below.

From a mathematical standpoint, the power of both the incremental and non-incremental Kolmogorov solution, (3) (or (4)) and (2), respectively, derives from the fact that these embody *representation theorems* [see, e.g., [9]] by which, in the present context, *any* entity, $\beta(\mathbf{p}, \omega)$, satisfying a generalized transport equation of the form $\beta_\omega + \mathbf{v} \cdot \nabla_{\mathbf{p}} \beta + \kappa \nabla_{\mathbf{p}}^2 \beta = F(\beta)$, and having an associated stochastic differential equation (SDE), $d\chi(\omega) = \mathbf{v}(\mathbf{p}, \omega) + \sqrt{2\kappa} d\mathbf{w}(\omega)$, can be determined in time-incremental fashion. Here, \mathbf{p} and ω represent variables that are, in the sense of this generalized transport equation, space- and time-like, respectively, \mathbf{v} and κ are, respectively, drift field and diffusion coefficient analogs, F is a generalized source term, and \mathbf{w} is a Wiener process.

From a physical standpoint, (3) and (4) likewise embody powerful features. In particular, since solutions of (1) via (3), or equivalently (4), require determination of the transition density p (or equivalently, $n(x'_i, \theta_{j+1})/(N\Delta x_i)$), where p typically captures short time- and length-scale physics, then in constructing solutions, we are immediately forced to confront physical features extant on these scales. In many continuum-scale scalar transport problems, for example, one can often reasonably assume that small scale statistical features are adequately captured by the Fokker-Planck, or somewhat more generally, the differential Chapman-Kolmogorov (CK) equation [16]. In

these cases, and again as illustrated in the first example below, due to the local nature of (3) or (4), p typically corresponds to a fundamental solution of the FP or CK equations. Similarly, in quantum-scale problems, where (3) (or (4)) corresponds to a time-incremental solution for a wave function, ψ , via a propagator U (see, e.g., [4]) (where ψ and U correspond respectively to η and p), one must typically construct a Hamiltonian appropriate to the quantum system of interest.

2. Example I: Cole-Hopf/KPZ transformation

In order to illustrate the utility of (3) (or (4)) in solving nonlinear problems, we choose two relatively simple embodiments of (1), the noise-free Burger's and KPZ equations, and show how the solution, (3), encompasses, and can be used to derive, the CH/KPZ transformations. Importantly, this exercise exposes two significant features. First, it illustrates a well known argument [8, 16] for obtaining a typical Gaussian transition density via solution of the FP equation; again, determination of p , either analytically by solution of the FP or CK equations, or by Monte Carlo simulation (leading to (4)) comprises the crucial step in solving (1) via (3) or (4).

Second, and reflecting what appears to be a new result, this exercise shows that in some cases, one can jump from a time-incremental solution, as in (3) or (4), to a non-incremental solution, as in the CH/KPZ transform solutions. The idea centers on circumventing a path integral, $E \int_{\theta_j}^{\theta_{j+1}} u(\chi(s'), s') ds'$, over an *a priori* unknown field, u , by first introducing a transformation $\phi(x', \theta) = \exp(f(u))$ into the representation (3), and then by insisting that the stochastic construction of ϕ be purely diffusive, i.e., that the stochastic process, $d\chi_\phi(s)$, used to construct ϕ be governed by $d\chi_\phi(s) = \sqrt{2}dw(s)$.

Thus, considering the noise-free Burger's equation, $u_\theta + uu_x + u_{xx} = 0$, we set $\eta = u$ in (3),

where, for hydrodynamic problems, u is the fluid velocity. The solution in (3) then takes the form

$$u(x, \theta_j) = \int_{-\infty}^{\infty} u(x', \theta_{j+1}) p(x, \theta_j | x', \theta_{j+1}) dx' \quad (5)$$

This is a time-incremental, stochastic solution to Burger's equation, and as far as we can determine, has not been reported.

In order to determine p : i) we again assume that the solution point (\mathbf{x}, θ) is far removed from both δQ and the final time slice $D \times \{\theta = T\}$, ii) again choose the time increment $\Delta\theta$ so that the local Reynolds number, or its equivalent, satisfies $Re_b = O(1)$, and iii) set the source term f in (1) to 0. Under these conditions, the transition density, $p(x, \theta_j | x', \theta_{j+1})$, can be determined explicitly using the backward Fokker-Planck equation, $p_\theta + u(x', \theta) p_{x'} + p_{x'x'} = 0$, subject to the condition $p(x, \theta_j | x', \theta_j) = \delta(x - x')$, with the result [8, 16]: $p(x, \theta_j | x', \theta_{j+1}) = [\sqrt{4\pi\Delta\theta}]^{-1} \exp -[(x' - \bar{x})^2 / (4\Delta\theta)]$, where again, $\bar{x} = x + E \int_{\theta_j}^{\theta_{j+1}} b(\chi(s'), s') ds'$ is the average position of the RW swarm at θ_{j+1} . Again, since $E \int_{\theta_j}^{\theta_{j+1}} u(\chi(s'), s') ds' = u(x, \theta_j) \Delta\theta + O(\Delta\theta^2)$, the presence of the path integral does not prevent time-incremental solutions; various strategies, involving, e.g., Taylor expansions relating the unknown $u(x, \theta_j)$ to known $u(x, \theta_{j+1})$, can be easily envisioned.

Next, arriving at the crucial step in the derivation of the Cole-Hopf solution, we take advantage of the general nature of (3), and as mentioned above, introduce a transformation

$$\phi(u) = \exp(f(u)) \quad (6)$$

into (3). Again, in order to circumvent the path integral over unknown u , we force the stochastic

construction of ϕ to be purely diffusive, $\phi_\theta + \phi_{xx} = 0$. Importantly, defining a purely diffusive ϕ of the form given in (6) allows us, on one hand, to stretch the solution interval to any arbitrary length (by eliminating the path integral), while on the other, providing us with sufficient freedom to identify transformations, $f(u)$, between the simple linear heat equation governing ϕ , and more complicated, nonlinear equations governing u . It appears likely that a similar strategy can be used to find long-time (non-incremental) transformations and solutions for other nonlinear equations.

Thus, recognizing that p is now governed by $p_\theta + p_{xx} = 0$, and inserting ϕ in (3), we obtain

$$\phi(x, \theta_j) = \int_{-\infty}^{\infty} \phi(x', \theta_{j+1}) \left[\sqrt{4\pi(\theta_{j+1} - \theta_j)} \right]^{-1} \exp -[(x' - x)^2 / (4(\theta_{j+1} - \theta_j))] dx' \quad (7)$$

where now $\bar{x} = x$.

At this stage, several equivalent paths can be taken to complete the derivation. The most transparent, which also provides the KPZ transform, first determines $f(u)$ by finding an equivalent transformation, $\phi = \phi(\tilde{f}(v))$, that solves the related *forward-time*, noise-free KPZ equation, $v_t + v_x^2/2 - v_{xx} = 0$. This is followed by use of the well-known transformation [17], $u = v_x$, between the KPZ and Burger's equations, after which ϕ is introduced into (3), θ_{j+1} stretched to the final backward time T , and the final result obtained.

Thus, the forward-time form of the governing equation for ϕ , $\phi_t - \phi_{xx} = 0$, yields $v_t - [\tilde{f}_v + \tilde{f}_{vv}/\tilde{f}_v]v_x^2 - v_{xx} = 0$, which, in turn, transforms to the KPZ equation by choosing $[\tilde{f}_v + \tilde{f}_{vv}/\tilde{f}_v] = -1/2$ (where we again set the coefficient multiplying v_{xx} to 1). Note, we change to a forward time solution for ϕ in order to obtain the correct signs on v . This is acceptable (and an advantage of this approach) since the purely diffusive stochastic process, χ_ϕ , used to construct ϕ can be run

in either the forward or backward time direction. In order to obtain a typical form of the KPZ transformation and solution [17], we choose $\tilde{f}_v = -1/2$, which then yields $\phi = \exp(-v/2)$, or $v(x, t) = -2 \ln \phi$, identical to the form given in [17] (with $\nu = 1$).

Next, restate ϕ in terms of u , $\phi = \exp[-1/2 \int^x u dx]$, and insert this into (3). Then isolate $u(x, \theta_j)$ using $u(x, \theta_j) = -2\phi_x/\phi|_{x, \theta_j}$, set $\theta_j = t$, $\theta_{j+1} = T$, and finally obtain, after some manipulation, the classic Cole-Hopf solution of Burger's equation (see, e.g., [12]):

$$u(x, t) = \frac{\int_{-\infty}^{\infty} \frac{(x-x')}{t} \exp(-G/2) dx'}{\int_{-\infty}^{\infty} \exp(-G/2) dx'} \quad (8)$$

where $G = G(x';, x, t) = \int_0^{x'} u(y, t = 0) dy + \frac{(x-x')^2}{2t}$.

3. Example II: Feynman-Kac formula

Turning next to solution of nonhomogeneous versions of (1) via (3), we illustrate by using (3) to derive the Feynman-Kac formula. In particular, consider a one-dimensional Schrödinger-like transport equation of the form $\eta_\theta + b\eta_x + \nu\eta_{xx} = V(x, \theta)\eta$, where b and ν either correspond to, or are local analogs to drift and diffusivity, and where V is a deterministic function. The Kolmogorov solution (3) over $\Delta\theta$ is thus stated as

$$\eta(x, \theta_j) = \int_{-\infty}^{\infty} p(x, \theta_j | x', \theta_{j+1}) \eta(x', \theta_{j+1}) dx' - E \int_{\theta_j}^{\theta_{j+1}} V(\chi(s'), s') \eta(\chi(s'), s') ds'. \quad (9)$$

For present purposes, there is no need to specify p . Thus, we first note that $E \int_{\theta_j}^{\theta_{j+1}} V(\chi(s'), s') \eta(\chi(s'), s') ds' = V(x, \theta_j) \eta(x, \theta_j) \Delta\theta + O(\Delta\theta^2)$. Hence, to $O(\Delta\theta^2)$, (9) can be expressed as

$\eta(x, \theta_j) = (1 + V\Delta\theta)^{-1} \int_{-\infty}^{\infty} p(x, \theta_j | x', \theta_{j+1}) \eta(x', \theta_{j+1}) dx'$, or, using $(1 + V\Delta\theta)^{-1} = (1 - V\Delta\theta) +$

$O(\Delta\theta^2) = \exp[-V(x, \theta_j)\Delta\theta] + O(\Delta\theta^2)$, as $\eta(x, \theta_j) = \exp[-V(x, \theta_j)\Delta\theta] \int_{-\infty}^{\infty} p(x, \theta_j|x', \theta_{j+1})\eta(x', \theta_{j+1})dx' + O(\Delta\theta^2)$.

Next, taking the expectation and suppressing the error estimate, we rewrite the preceding expression for $\eta(x, \theta_j)$ as $\eta(x, \theta_j) = \exp[-V(x, \theta_j)\Delta\theta]\eta(\bar{x}_{j+1}, \theta_{j+1})$, where the average position of the RW swarm at θ_{j+1} is expressed as \bar{x}_{j+1} . With this last expression, we can now connect $\eta(x, \theta_j)$ to $\eta(\bar{x}_N, \theta_N)$, the value of η in the final time-slice $D \times \{\theta = T\}$, evaluated at the swarm's final mean position, \bar{x}_N ; thus, $\eta(x, \theta_j) = \exp \left[-\Delta\theta [V(x, \theta_j) + V(\bar{x}_{j+1}, \theta_{j+1}) + V(\bar{x}_{j+2}, \theta_{j+2}) + \dots + V(\bar{x}_N, \theta_N)] \right] \eta(\bar{x}_N, \theta_N)$, or finally, $\eta(x, \theta_j) = E \left[\exp \left[-\int_{\theta_j}^{\theta_N} V(\chi(s'), s')ds' \right] \right] \eta(\bar{x}_N, \theta_N)$.

A closing note regarding nonhomogeneous problems: as before, in cases where an analytical solution for the transition density, p , cannot be obtained, then an incremental stochastic construction can be carried out using an appropriate SDE combined with the approximate representation in (4). In the present illustration, for example, the stochastic processes used to construct η are governed by $d\chi(\theta) = b(\chi(\theta), \theta)d\theta + \sqrt{2\nu}dw(\theta)$.

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